Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

[4-Bromo-2-(pyridin-2-ylmethyliminomethyl)-phenolato]methanolperchloratozinc(II)

Yi-Jun Wei

Department of Chemistry, Huainan Normal College, Huainan 232001, People's Republic of China

Correspondence e-mail: huainanweiyijun@163.com

Received 7 April 2005
Accepted 22 April 2005
Online 14 May 2005

Key indicators

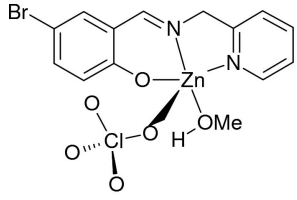
Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.007 Å
Disorder in main residue
R factor = 0.048
wR factor = 0.129
Data-to-parameter ratio = 14.9

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

In the title mononuclear zinc(II) compound, $[Zn(C_{13}H_{10}BrN_2O)(ClO_4)(CH_4O)]$, the Zn^{II} ion is in a square-pyramidal geometry, and is coordinated in the basal plane by an O atom and two N atoms from a Schiff base ligand and an O atom from the coordinated MeOH molecule. The apical position is occupied by an O atom from a perchlorate anion. In the crystal structure, the molecules form hydrogen-bonded dimers *via* the methanol hydroxy group and the phenolate O atom of a symmetry-related molecule. They are further linked by C—H···O interactions, *via* the perchlorate O atoms, forming a network structure.

Comment

Zinc complexes are very important in biology, functioning as the active site of hydrolytic enzymes, where they are in a hard-donor coordination environment of nitrogen and oxygen (Sanmartín *et al.*, 2000; Vallee & Auld, 1993). In order to investigate the structures of such zinc compounds, the title mononuclear zinc(II) complex, (I), was synthesized and its structure is reported here.



(I)

The molecular structure of complex (I) is illustrated in Fig. 1. Selected bond distances and angles are given in Table 1. The Zn^{II} ion is in a square-pyramidal geometry, and is

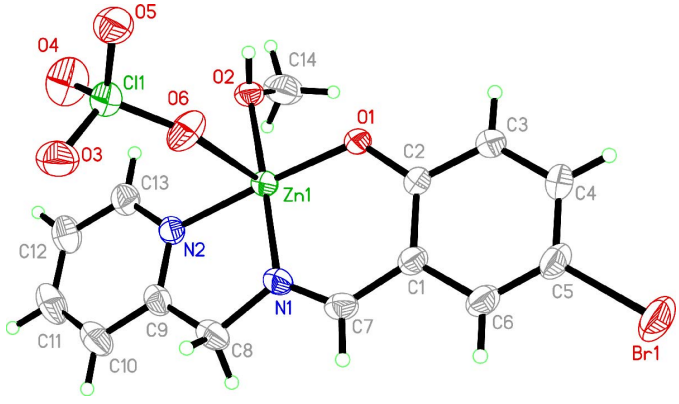


Figure 1
The molecular structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. Only the major component of the disordered perchlorate ligand is shown.

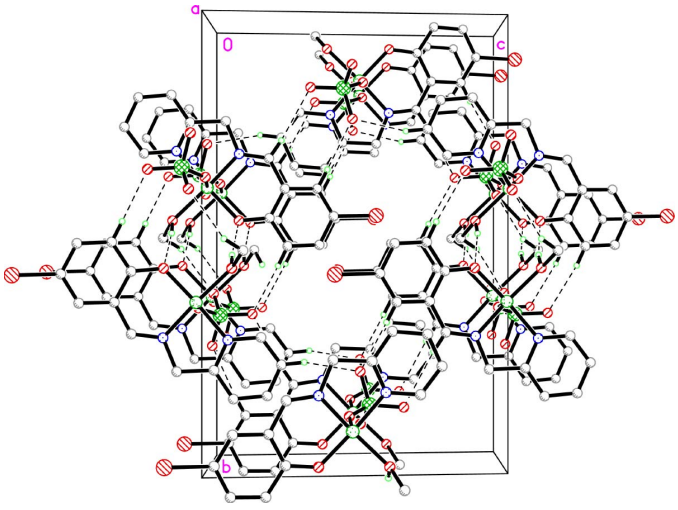


Figure 2
The crystal packing of (I), viewed along the *a* axis. Dashed lines indicate hydrogen bonds. The H atoms not involved in the hydrogen bonds have been omitted for clarity. Only the major disorder component is shown.

coordinated in the basal plane by atoms O1, N1 and N2 from the Schiff base ligand and atom O2 of the coordinated MeOH molecule. The apical position is occupied by atom O6 from a perchlorate anion. All the bond lengths are in normal ranges (Allen *et al.*, 1987). The bond lengths involving the Zn^{II} ion are comparable with the corresponding values observed in other zinc(II) complexes (McCleverty *et al.*, 1980; Usman *et al.*, 2003). The two *trans* bond angles in the basal plane are 176.50 (13) and 175.08 (13)°. All the other bond angles at the Zn^{II} ion are close to 90°, ranging from 83.00 (14) to 93.65 (13)°. The bond angle N1—Zn1—N2 deviates from 90° by 7.00 (14)°, which is due to the strain created by the five-membered chelate ring Zn1/N1/C8/C9/N2.

In the crystal structure, the molecules form hydrogen-bonded dimers *via* the methanol hydroxy group and atom O1 of a symmetry-related molecule (Table 2 and Fig. 2). They are further linked by C—H···O interactions, *via* the perchlorate O atoms, forming a network structure.

Experimental

Salicylaldehyde (0.2 mmol, 24.3 mg) and 2-aminomethylpyridine (0.2 mmol, 21.5 mg) were dissolved in MeOH (15 ml). The mixture was stirred for about 30 min to give a clear yellow solution. To the solution was added an MeOH solution (15 ml) of $Zn(ClO_4)_2{\cdot}7H_2O$ (0.1 mmol, 39.1 mg), with stirring. After keeping the resulting colourless solution in air for 13 d, colourless block-shaped crystals were formed.

Crystal data

$[Zn(C_{13}H_{10}BrN_2O)(ClO_4)(CH_4O)]$
M_r = 487.00
Monoclinic, $P2_1/n$
a = 7.207 (3) Å
b = 19.112 (4) Å
c = 12.686 (3) Å
β = 95.67 (3)°
V = 1738.8 (9) Å^3
Z = 4
D_x = 1.860 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 3436 reflections
θ = 2.7–23.4°
μ = 3.90 mm^{-1}
T = 298 (2) K
Block, colourless
0.17 × 0.14 × 0.13 mm

Data collection

Bruker SMART CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.557, T_{max} = 0.631
14 781 measured reflections
3968 independent reflections
2916 reflections with $I > 2\sigma(I)$
R_{int} = 0.033
θ_{max} = 27.5°
$h = -9 \rightarrow 9$
$k = -24 \rightarrow 24$
$l = -16 \rightarrow 16$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.129
S = 1.04
3968 reflections
267 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0565P)^2 + 1.9852P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 1.13 e Å^{-3}
$\Delta\rho_{min}$ = −0.53 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Zn1—O1	1.901 (3)	Zn1—O2	1.987 (3)
Zn1—N1	1.934 (3)	Zn1—O6	2.483 (8)
Zn1—N2	1.981 (3)		
O1—Zn1—N1	93.63 (13)	N2—Zn1—O2	93.65 (13)
O1—Zn1—N2	176.50 (13)	O1—Zn1—O6	92.0 (2)
N1—Zn1—N2	83.00 (14)	N1—Zn1—O6	89.9 (4)
O1—Zn1—O2	89.78 (12)	N2—Zn1—O6	87.1 (2)
N1—Zn1—O2	175.08 (13)	O2—Zn1—O6	93.6 (4)

Table 2
Hydrogen-bonding geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O2—H2···O1^{i}	0.84 (4)	1.86 (4)	2.679 (4)	165 (6)

Symmetry code: (i) $1-x, -y, 1-z$.

The O atoms of the perchlorate ligand are disordered over two distinct sites, with occupancies of 0.522 (8) and 0.478 (8). The Cl—O and O···O distances in both disordered components were restrained to be equal. The methanol hydroxyl H atom was located in a difference Fourier map and refined isotropically, with the O—H distance restrained to 0.84 (1) Å. The other H atoms were placed in idealized positions and constrained to ride on their parent atoms, with C—H distances in the range 0.93–0.97 Å, and with U_{iso}(H) = 1.2 or 1.5U_{eq}(C). An unassigned maximum residual density was observed 0.88 Å from atom Br1.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

The author thanks the Education Office of Anhui Province, People's Republic of China, for research grant No. 2004kj326.

References

Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans.* 2, pp. S1–83.

Bruker (1998). *SMART* (Version 5.628) and *SAINT* (Version 6.02). Bruker AXS Inc., Madison, Wisconsin, USA.
McCleverty, J. A., Morrison, N. J., Spencer, N., Ashworth, C. C., Bailey, N. A., Johnson, M. R., Smith, J. M. A., Tabbiner, B. A. & Taylor, C. R. (1980). *J. Chem. Soc. Dalton Trans.* pp. 1945–1957.
Sanmartín, J., Bermejo, M. R., García-Deibe, A. M., Rivas, I. M. & Fernández, A. R. (2000). *J. Chem. Soc. Dalton Trans.* pp. 4174–4181.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997*a*). *SHELXL97* and *SHELXS97*. University of Göttingen, Germany.
Sheldrick, G. M. (1997*b*). *SHELXTL*. Version 5.1. Bruker AXS Inc., Madison, Wisconsin, USA.
Usman, A., Fun, H.-K., Chantrapromma, S., Zhu, H.-L. & Liu, Q.-X. (2003). *Acta Cryst.* E**59**, o215–o217.
Vallee, B. L. & Auld, D. S. (1993). *Acc. Chem. Res.* **26**, 543–551.